

# 1 ML twin refinement, a slightly different approach

## 1.1 Notation

- $F_{\mathbf{H}_{a,t}}$ : The true, error free structure factor amplitude with index  $\mathbf{H}_a$ .
- $F_{\mathbf{H}_{b,t}}$ : The true, error free structure factor amplitude with index  $\mathbf{H}_b$ .
- $F_{\mathbf{H}_{a,c}}$ : The calculated structure factor amplitude with index  $\mathbf{H}_a$ .
- $F_{\mathbf{H}_{b,c}}$ : The calculated structure factor amplitude with index  $\mathbf{H}_b$ .
- $F_{\mathbf{H}_{a,o}}$ : The observed structure factor amplitude with index  $\mathbf{H}_a$ .
- $F_{\mathbf{H}_{b,o}}$ : The observed structure factor amplitude with index  $\mathbf{H}_b$ .

Other variables for twinned intensities ( $J$ ), or ‘plain’ intensities ( $I$ ) follow the same subscripts (t,c,o) . The twin fraction is denoted with  $\tau$ , due to the use of  $\alpha, \beta$  notation in likelihoods.

## 1.2 Basic likelihood function

The standard likelihood function has the following form:

$$P(F_{\mathbf{H}_{a,t}}|F_{\mathbf{H}_{a,c}}) = \frac{2F_{\mathbf{H}_{a,t}}}{\beta} \exp \left[ -\frac{F_{\mathbf{H}_{a,t}}^2 + \alpha F_{\mathbf{H}_{a,c}}^2}{\beta} \right] I_0 \left[ \frac{2\alpha F_{\mathbf{H}_{a,t}} F_{\mathbf{H}_{a,c}}}{\beta} \right] \quad (1)$$

Assuming independence between reflections, one can write

$$P(F_{\mathbf{H}_{a,t}} F_{\mathbf{H}_{a,t}} | F_{\mathbf{H}_{a,c}} F_{\mathbf{H}_{b,c}}) = P(F_{\mathbf{H}_{a,t}} | F_{\mathbf{H}_{a,c}}) P(F_{\mathbf{H}_{b,t}} | F_{\mathbf{H}_{b,c}}) \quad (2)$$

Previous derivations took this equation and transformed variables  $F_{\mathbf{H}_{a,t}}$  and  $F_{\mathbf{H}_{b,t}}$  first to intensities and at a later stage to twinned intensities. I think I have an easier way of introducing twinning, which is related to how experimental errors are introduced into a likelihood function. A minor detour is taken that was instructive for myself.

### 1.3 A minor detour

Try to introduce experimental errors like this (note the use of intensities) :

$$P(I_{\mathbf{H}_{a,o}}|I_{\mathbf{H}_{a,t}}) = \frac{1}{\sqrt{2\pi}\sigma_a} \exp \left[ -\frac{(I_{\mathbf{H}_{a,o}} - I_{\mathbf{H}_{a,t}})^2}{2\sigma_a^2} \right] \quad (3)$$

Since  $I_{\mathbf{H}_{a,t}}$  is not a random variable, we can reparametrise at will ( $I_{\mathbf{H}_{a,t}} = F_{\mathbf{H}_{a,t}}^2$ ) and do not need to introduce a Jacobian:

$$P(I_{\mathbf{H}_{a,o}}|F_{\mathbf{H}_{a,t}}) = \frac{1}{\sqrt{2\pi}\sigma_a} \exp \left[ -\frac{(I_{\mathbf{H}_{a,o}} - F_{\mathbf{H}_{a,t}}^2)^2}{2\sigma_a^2} \right] \quad (4)$$

and thus

$$P(I_{\mathbf{H}_{a,o}}|F_{\mathbf{H}_{a,c}}) = \int_0^\infty P(I_{\mathbf{H}_{a,o}}|F_{\mathbf{H}_{a,t}}) P(F_{\mathbf{H}_{a,t}}|F_{\mathbf{H}_{a,c}}) dF_{\mathbf{H}_{a,t}} \quad (5)$$

$$= \int_0^\infty P(I_{\mathbf{H}_{a,o}}|F_{\mathbf{H}_{a,t}}) P(F_{\mathbf{H}_{a,t}}|F_{\mathbf{H}_{a,c}}) dF_{\mathbf{H}_{a,t}} \quad (6)$$

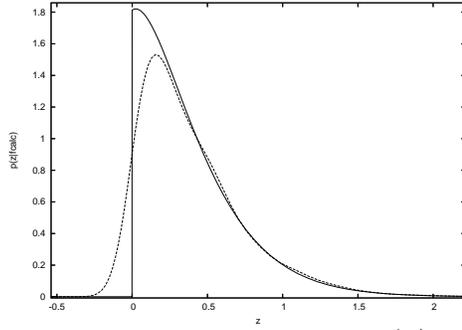
Approximate the integral with a quadrature:

$$P(I_{\mathbf{H}_{a,o}}|F_{\mathbf{H}_{a,c}}) = \sum_{j=0}^{j<N} w[j] P(I_{\mathbf{H}_{a,o}}|F_{\mathbf{H}_{a,t}}[j]) P(F_{\mathbf{H}_{a,t}}[j]|F_{\mathbf{H}_{a,c}}) \quad (7)$$

Where the weights  $w[j]$  and the nodes  $F_{\mathbf{H}_{a,t}}[j]$  will have to be determined. Strategic placement of nodes and weights will probably require some care. Of course, a Laplace approximation could be used as well. It is not clear to me how to take care of target function derivatives when using a Laplace approximation.

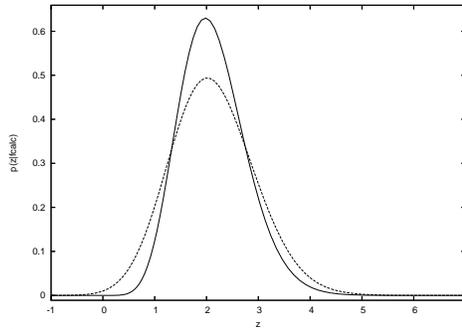
#### 1.3.1 An example

Set  $\alpha$  to 0.90 and  $\beta$  to 0.19,  $F_{\mathbf{H}_{a,c}}$  to 0.5 and  $\sigma_a$  to 0.1. This gives



The continuous line is the  $P(z|F_{\mathbf{H}_{a,c}})$  without taking into account experimental error. The striped line is when the error are taken into account.

Setting  $\alpha$  to 0.95 and  $\beta$  to 0.1,  $F_{\mathbf{H}_{a,c}}$  to 1.5 and  $\sigma_a$  to 0.5 gives:



Striped and continuous lines are as above. In both cases, integrations were carried out with a (brute force) low discrepancy Halton sequence with 400 points. A more careful integration using an appropriate quadrature can significantly reduce the number of nodes that need to be sampled. If the maximum value of the integrand is found, one can choose the region in which one integrates to be in the area where the integrand has the largest mass. Initial results using a Gauss-Legendre quadrature are encouraging.

## 1.4 Twinned data

With the insights of the one dimensional case, we can say

$$P(J_{\mathbf{H}_{a,o}} J_{\mathbf{H}_{b,o}} | J_{\mathbf{H}_{a,t}} J_{\mathbf{H}_{b,t}}) = \frac{1}{2\pi\sigma_a\sigma_b} \exp \left[ -\frac{(J_{\mathbf{H}_{a,o}} - J_{\mathbf{H}_{a,t}})^2}{2\sigma_a^2} - \frac{(J_{\mathbf{H}_{b,o}} - J_{\mathbf{H}_{b,t}})^2}{2\sigma_b^2} \right] \quad (8)$$

Introduce twinning:

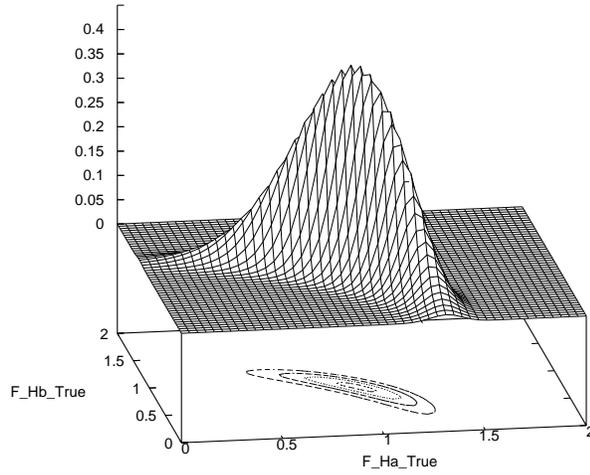
$$J_{\mathbf{H}_{a,t}} = (1 - \tau)F_{\mathbf{H}_{a,t}}^2 + \tau F_{\mathbf{H}_{b,t}}^2 \quad (9)$$

$$J_{\mathbf{H}_{b,t}} = \tau F_{\mathbf{H}_{a,t}}^2 + (1 - \tau)F_{\mathbf{H}_{b,t}}^2 \quad (10)$$

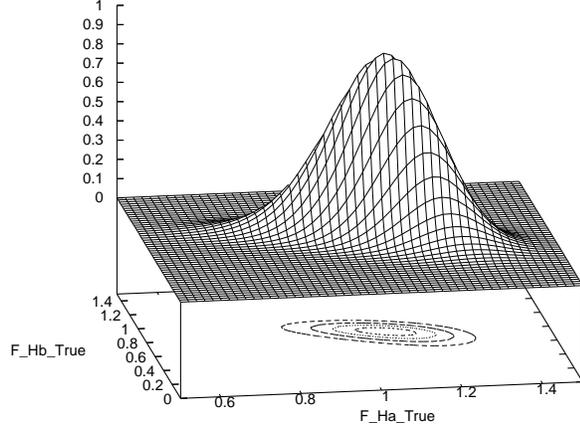
and obtain  $P(J_{\mathbf{H}_{a,o}}J_{\mathbf{H}_{b,o}}|F_{\mathbf{H}_{a,t}}F_{\mathbf{H}_{b,t}})$ , to bring

$$P(J_{\mathbf{H}_{a,o}}J_{\mathbf{H}_{b,o}}|F_{\mathbf{H}_{a,c}}F_{\mathbf{H}_{b,c}}) = \int_0^\infty \int_0^\infty P(J_{\mathbf{H}_{a,o}}J_{\mathbf{H}_{b,o}}|F_{\mathbf{H}_{a,t}}F_{\mathbf{H}_{b,t}}) \times P(F_{\mathbf{H}_{a,t}}F_{\mathbf{H}_{b,t}}|F_{\mathbf{H}_{a,c}}F_{\mathbf{H}_{b,c}})dF_{\mathbf{H}_{a,t}}dF_{\mathbf{H}_{b,t}} \quad (11)$$

Note the absence of singularities when the twin fraction is a half: no 'detwinning' is involved that would be result of changing variables in  $P(F_{\mathbf{H}_{a,t}}F_{\mathbf{H}_{b,t}}|F_{\mathbf{H}_{a,c}}F_{\mathbf{H}_{b,c}})$  to describe twinning. Approximating  $P(F_{\mathbf{H}_{a,t}}F_{\mathbf{H}_{b,t}}|F_{\mathbf{H}_{a,c}}F_{\mathbf{H}_{b,c}})$  with a Gaussian, the integrant in expression 11 looks like a 2D Gaussian, albeit it bit 'curvy':



In the previous figure, the twin fraction was set to a half. When the twin fraction is less than a half, more Gaussian like integrants appear: in the next figure the twin fraction was set to 0.25:



Although these figures do not prove anything, they do indicate that approximating the integral 11 with a quadrature, would provide a relatively straightforward approximation:

$$\begin{aligned}
 P(J_{\mathbf{H}_{a,o}} J_{\mathbf{H}_{b,o}} | F_{\mathbf{H}_{a,c}} F_{\mathbf{H}_{b,c}}) &= \sum_i \sum_j w[i] w[j] P(J_{\mathbf{H}_{a,o}} J_{\mathbf{H}_{b,o}} | F_{\mathbf{H}_{a,t}}[j] F_{\mathbf{H}_{b,t}}[j]) \times \\
 &P(F_{\mathbf{H}_{a,t}}[j] F_{\mathbf{H}_{b,t}}[j] | F_{\mathbf{H}_{a,c}} F_{\mathbf{H}_{b,c}})
 \end{aligned}
 \tag{12}$$